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Mathematical Modeling of the Role of Chemical Speciation on Electrokinetic Transport of Chemicals in Soil

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The efficiency of the electrokinetic remediation of heavy metal polluted soil is been demonstrated to be dependent upon the chemical reactivity of the target contaminant rather than the migration rate of the target ions. The contaminants have to be in a soluble species, preferably as ionic form, in order to be mobilized under the gradient of electrical potential induced in the system.

In the present work, a mathematical model for chemical equilibrium calculation is developed and used for the analysis of the interactions between the species in the pore solution and the solid matrix in lead contaminated soil. The model is based on the simultaneous solution of a non-linear set of reversible aqueous and precipitation/dissolution chemical reactions. A line search Newton-Raphson method, iterating on the extent of each reaction, is used for the chemical equilibrium calculations.

Simulations are presented in order to show the behavior of the chemical system with respect to the buffering capacity of the soil and the pH changes of the pore solution induced by the electrode reactions in the electrochemical treatment. Additionally, the role of some extracting agents in the speciation of lead is discussed. Results from simulations shed light on the effect of the speciation of lead in soil in the transport process, and can be useful for a correct design of enhanced electrokinetic remediation treatments.

Juan Manuel Paz-Garcia obtained his M.Sc. in Chemical Engineering, at the University of Málaga, Spain. He is currently a Ph.D. student at the Civil Engineering Department of the Technical University of Denmark, participating in a Ph.D. project named "Chemical and Numerical Modeling of Electrokinetics". Recently, Juan Manuel is a guest visiting scholar at the Civil and Environmental Engineering department, Northeastern University, Boston.